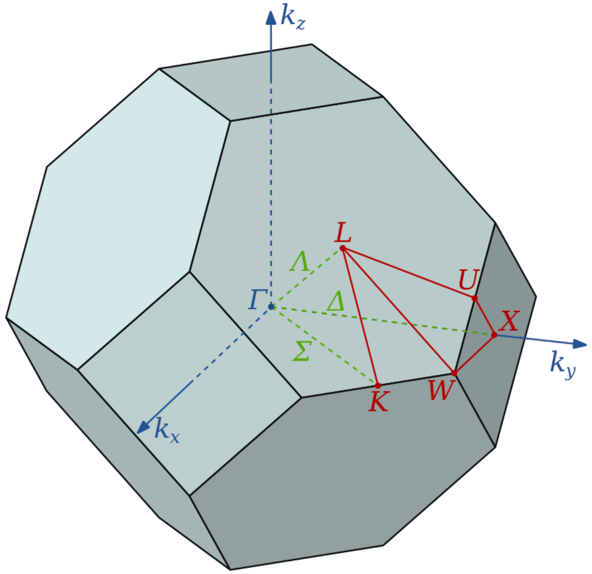
Special Topics on Basic EECS I
VLSI Devices
Lecture 3

Sung-Min Hong (smhong@gist.ac.kr)
Semiconductor Device Simulation Laboratory
School of Electrical Engineering and Computer Science
Gwangju Institute of Science and Technology

Velocity and inverse mass



- Velocity

$$\mathbf{v}(\mathbf{k}) = \frac{1}{\hbar} \nabla_k E(\mathbf{k})$$

- Inverse mass (its ij component)

$$m_{ij}^{-1} = \frac{1}{\hbar^2} \frac{\partial}{\partial k_i} \frac{\partial}{\partial k_j} E(\mathbf{k})$$

- Example) Silicon conduction band

$$E(\mathbf{k}) - E_c = \frac{\hbar^2}{2} \left(\frac{1}{m_{xx}} k_x^2 + \frac{1}{m_{yy}} k_y^2 + \frac{1}{m_{zz}} k_z^2 \right)$$ ~ Taur, Eq. (2.2)

  – Among three masses, one is m_l and the other two are m_t.

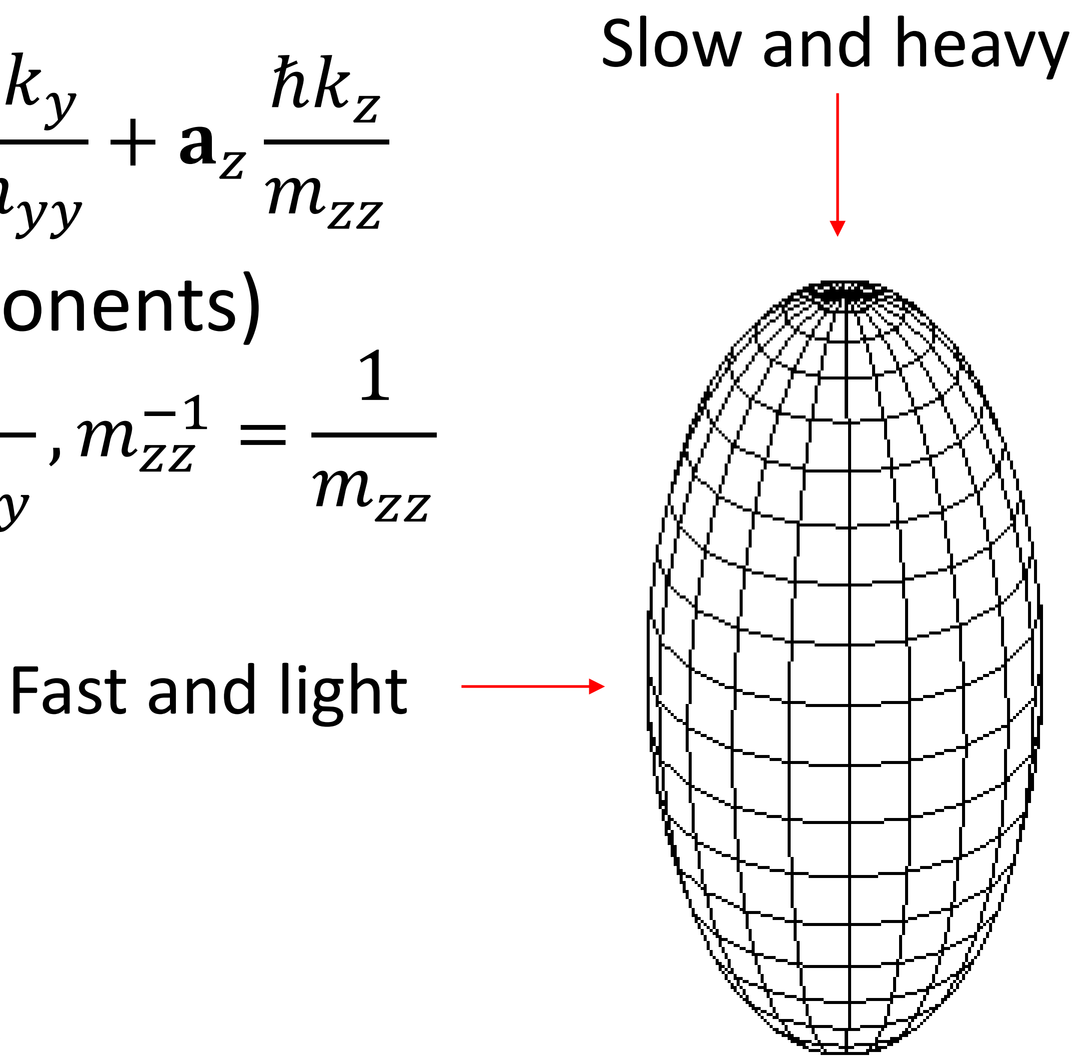
$\mathbf{v}$ and m^{-1} of an ellipsoidal valley

- Velocity

$$\mathbf{v}(\mathbf{k}) = \mathbf{a}_x \frac{\hbar k_x}{m_{xx}} + \mathbf{a}_y \frac{\hbar k_y}{m_{yy}} + \mathbf{a}_z \frac{\hbar k_z}{m_{zz}}$$

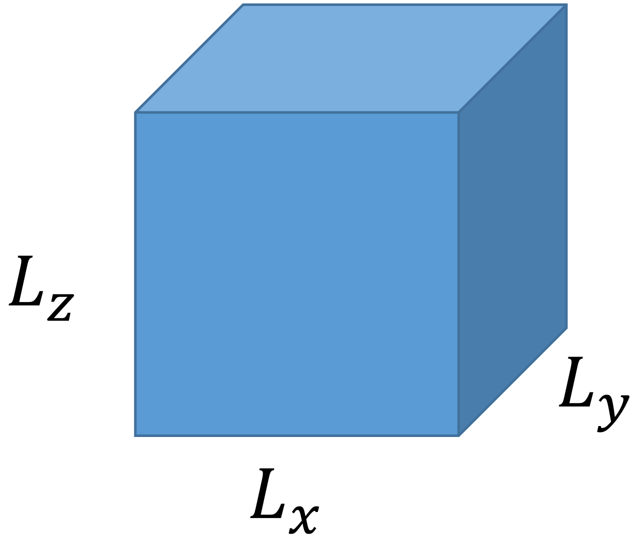
- Inverse mass (non-vanishing components)

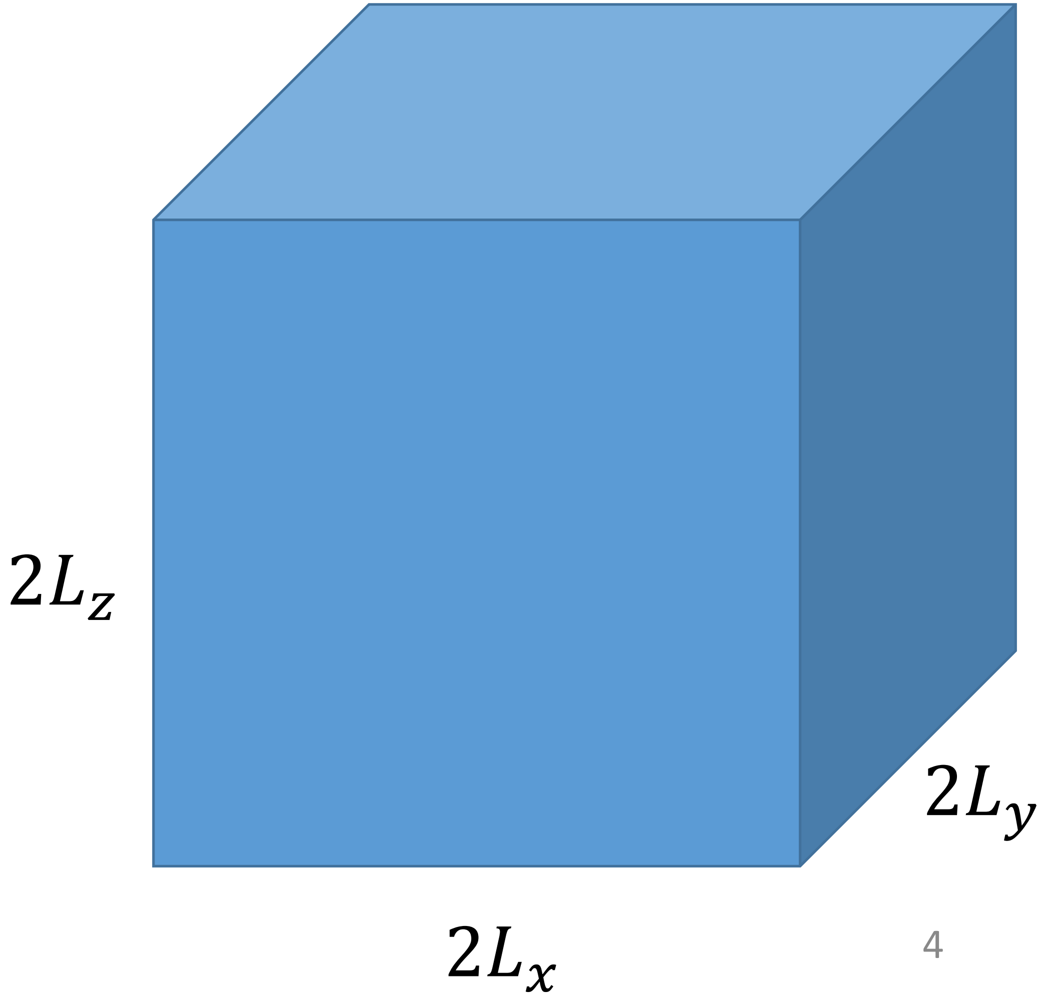
$$m_{xx}^{-1} = \frac{1}{m_{xx}}, m_{yy}^{-1} = \frac{1}{m_{yy}}, m_{zz}^{-1} = \frac{1}{m_{zz}}$$



Volume of a state in the $\mathbf{k}$-space

- A (discrete) $\mathbf{k}$ point corresponds to an electronic state.
  - One state within $\frac{(2\pi)^3}{L_x L_y L_z}$ (Left)
  - One state within $\frac{(2\pi)^3}{8 L_x L_y L_z}$ (Right)
  - In general, one state within $\frac{(2\pi)^3}{Volume}$





Number of states inside $\boldsymbol{dk_x dk_y dk_z}$

- Since a state takes $\frac{(2\pi)^3}{Volume}$,
  - Number of states inside $dk_x dk_y dk_z$ is

$$\frac{Volume}{(2\pi)^3} dk_x dk_y dk_z$$

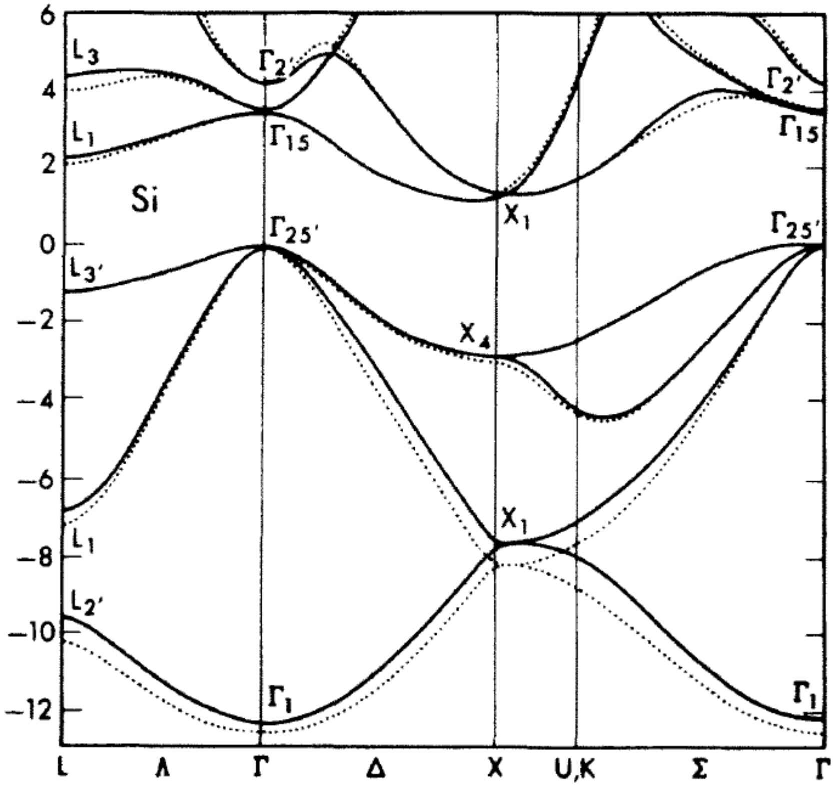
  - Number of states inside a range of $[E, E + dE]$,

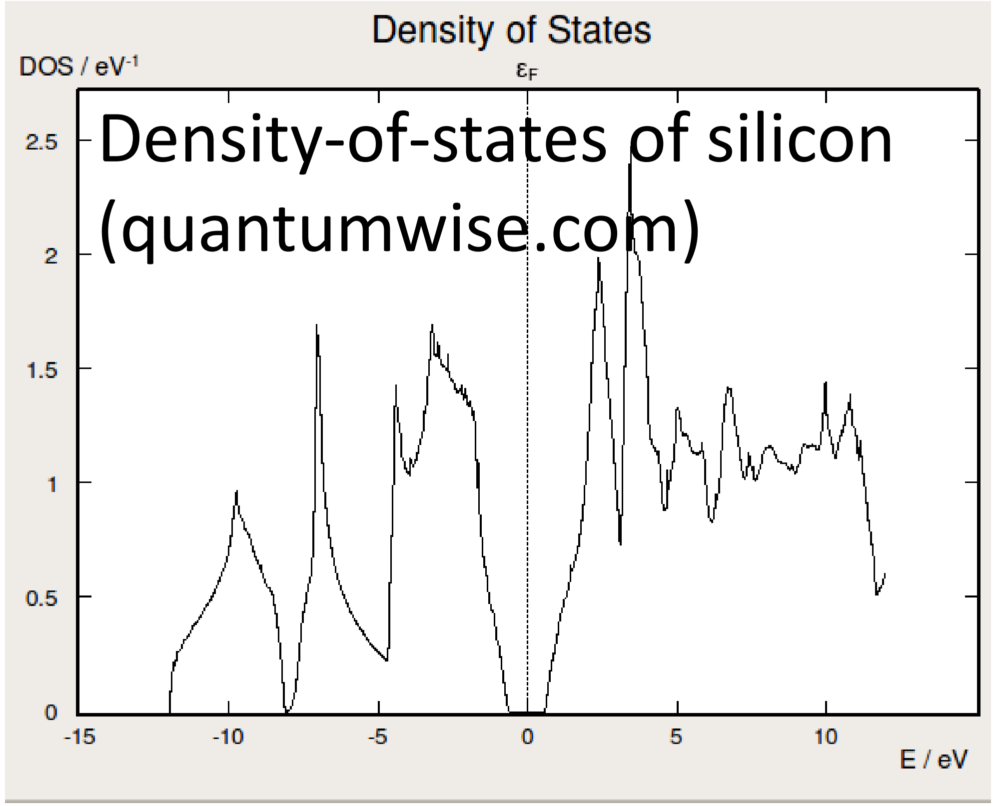
$$\frac{Volume}{(2\pi)^3} \iiint_{E(\mathbf{k}) \in [E, E+dE]} dk_x dk_y dk_z$$

Density-of-states (DOS)

- DOS, $N(E)$, (per spin, per valley)

$$N(E)dE = \frac{1}{(2\pi)^3} \iiint_{E(\mathbf{k})\in(E,E+dE)} dk_x dk_y dk_z \qquad \text{~ Taur, Eq. (2.1)}$$





Density-of-states of silicon (quantumwise.com)

Density-of-states (DOS) of an ellipsoidal valley

- Volume in the $\mathbf{k}$-space
  - With $m^* = \left(m_{xx}m_{yy}m_{zz}\right)^{\frac{1}{3}}$,

$$\frac{4\pi}{3}\left(\frac{1}{\hbar}\right)^3 (2m^*)^{1.5}(E-E_c)^{1.5}$$

  - Therefore, within a range between $E-E_c$ and $E-E_c+dE$,

$$4\pi\left(\frac{1}{\hbar}\right)^3 \left(2m_{xx}m_{yy}m_{zz}\right)^{0.5}(E-E_c)^{0.5}dE$$

- DOS of silicon conduction band (per spin, per valley)

$$N(E)dE = \frac{4\pi}{h^3}(2m_l m_t^2)^{0.5}(E-E_c)^{0.5}dE$$ ~ Taur, Eq. (2.3)

Homework#1

- Non-parabolicity, α
  - Consider an isotropic valley,

$$E(1+\alpha E)=\frac{\hbar^2}{2m^*}k^2$$

  - For this valley, express the velocity, the inverse mass, and the DOS using E.

Electron density

0, when empty
1, when occupied

- Number of electrons

$$\# = \sum_{\substack{all\ \textcolor{red}{occupied} \\ \mathbf{k}\ states}} 1 = \sum_{all\ \mathbf{k}\ states} f(\mathbf{k})$$

  - Instead of a sum,

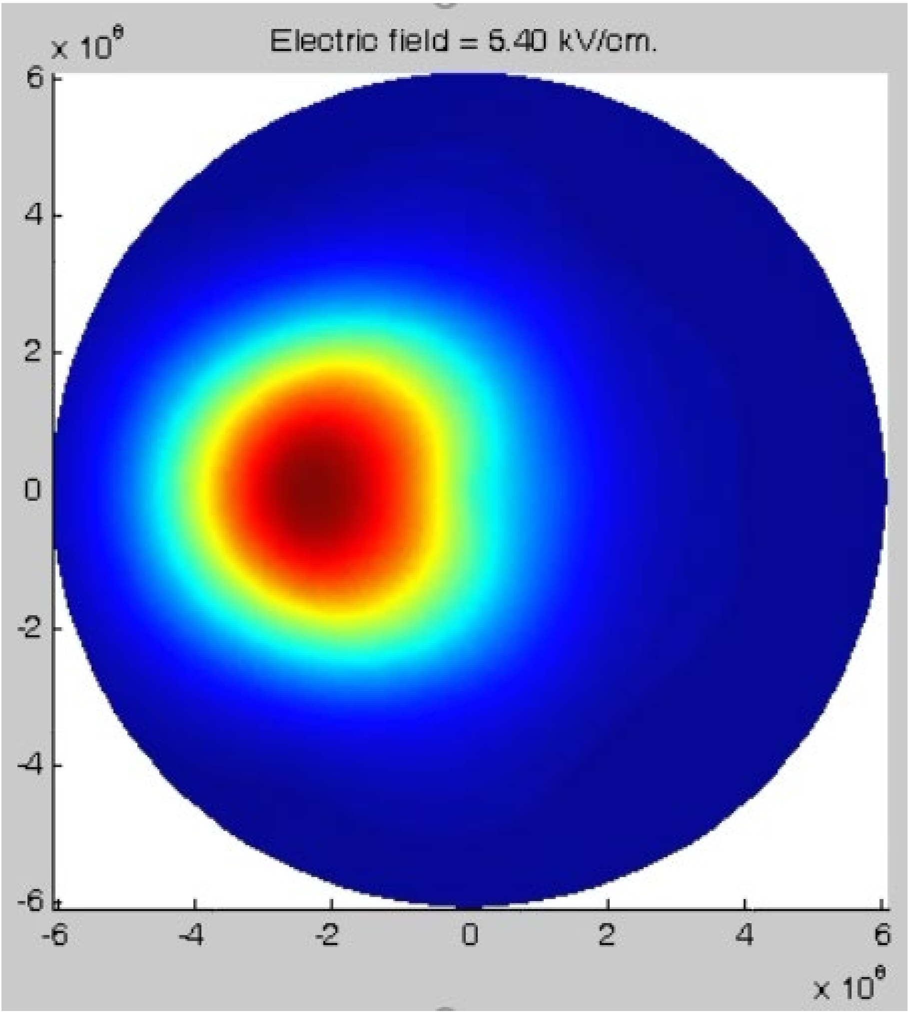
$$\# = \sum_{all\ \mathbf{k}\ states} f(\mathbf{k}) \approx \frac{Volume}{(2\pi)^3} \iiint_{\substack{Entire \\ \mathbf{k}\ space}} f(\mathbf{k}) dk_x dk_y dk_z$$

  - Electron density (per spin, per valley)

$$n = \frac{\#}{Volume} = \frac{1}{(2\pi)^3} \iiint_{\substack{Entire \\ \mathbf{k}\ space}} f(\mathbf{k}) dk_x dk_y dk_z$$

Distribution function

- $f(\mathbf{k})$ is the distribution function.
  - It is 0, when the state is completely empty.
  - It is 1, when the state is fully occupied.
  - It is in a range of [0,1].
  - In general, it is a function of $\mathbf{k}$.



Distribution function of graphene at a high electric field

A special case

- Sometimes, $f(\mathbf{k})$ depends on only the energy, $f(E)$.
  - In such a case, the electron density can be written as

$$n = \frac{1}{(2\pi)^3} \iiint\limits_{\substack{Entire \\ \mathbf{k}\, space}} f(\mathbf{k}) dk_x dk_y dk_z = \int_{E_C}^{\infty} N(E) f(E) dE$$

~ Taur, Eq. (2.7)

  - When do we have $f(E)$, instead of $f(\mathbf{k})$?
  - The equilibrium state is a typical example.

Fermi-Dirac distribution

- At equilibrium, the Fermi-Dirac distribution holds

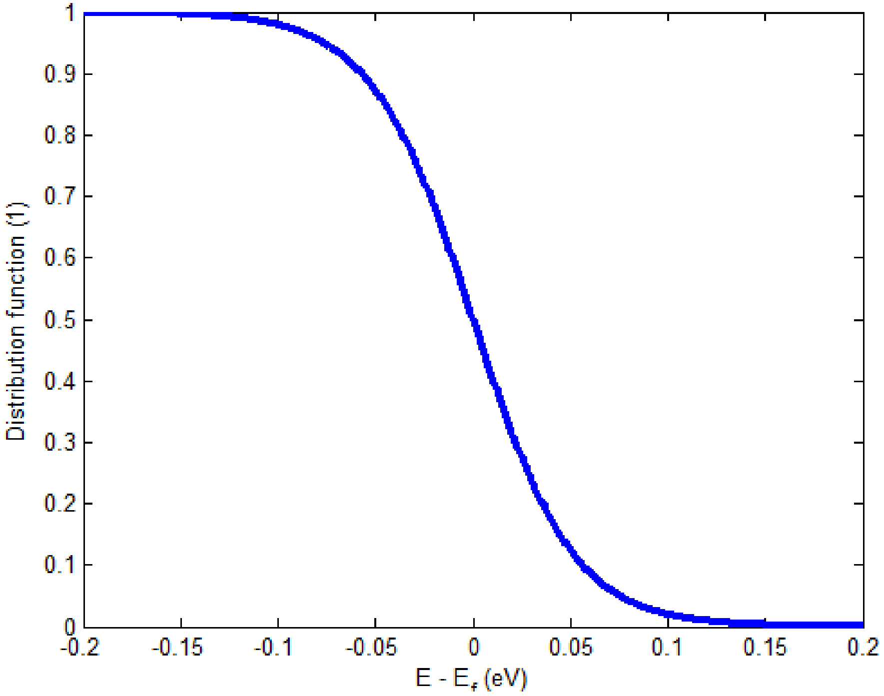
$$f_D(E) = \frac{1}{1 + \exp\left(\frac{E - E_f}{k_B T}\right)}$$

Taur, Eq. (2.4)

~ 0.02585 meV
@ 300 K

  - At $E = E_f$ (Fermi level),

$$f_D(E_f) = \frac{1}{2}$$

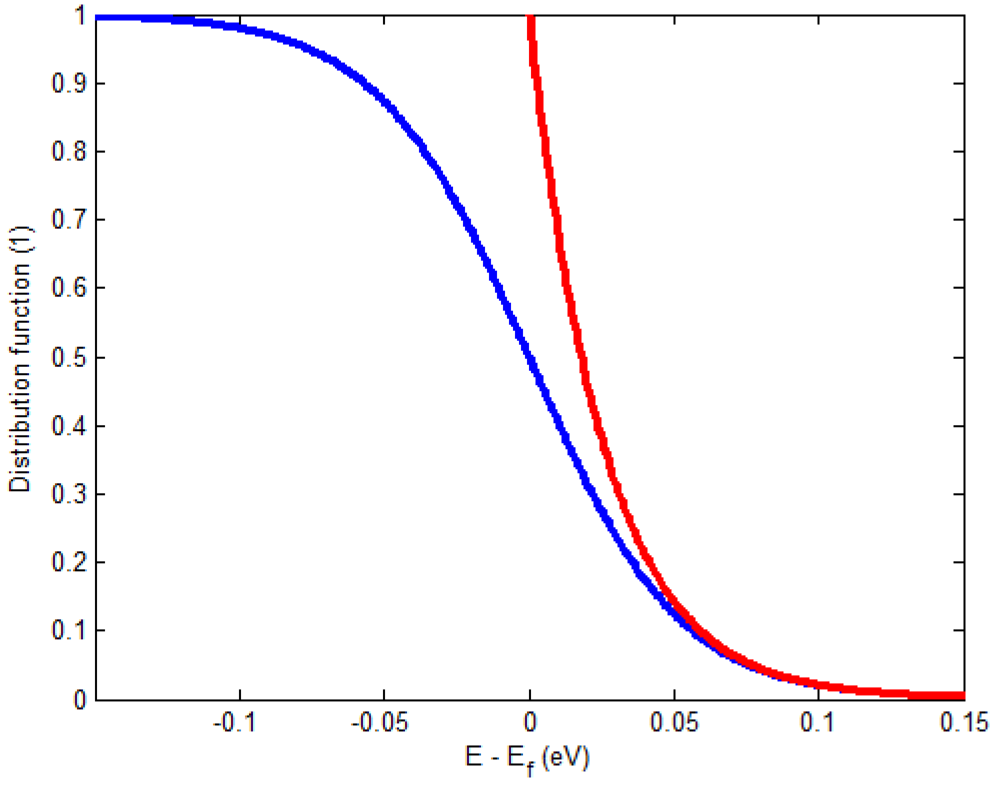


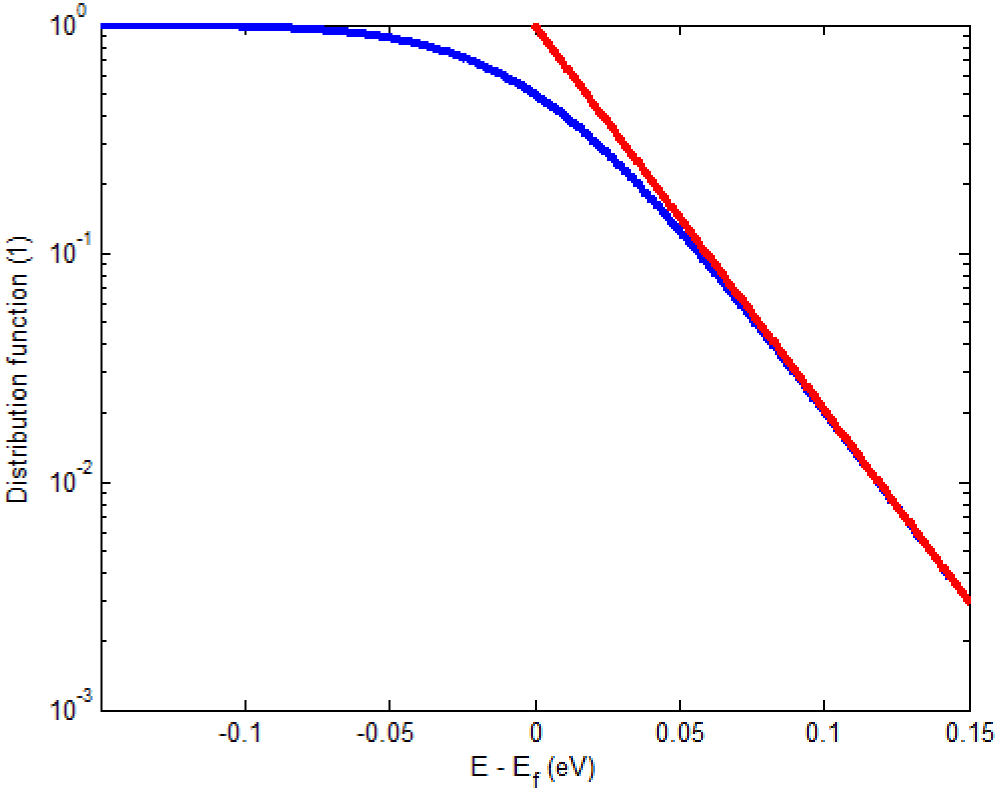
Boltzmann limit

- When $E > E_f$,

$$f_D(E) \approx \exp\left(-\frac{E - E_f}{k_B T}\right)$$

Taur, Eq. (2.5)



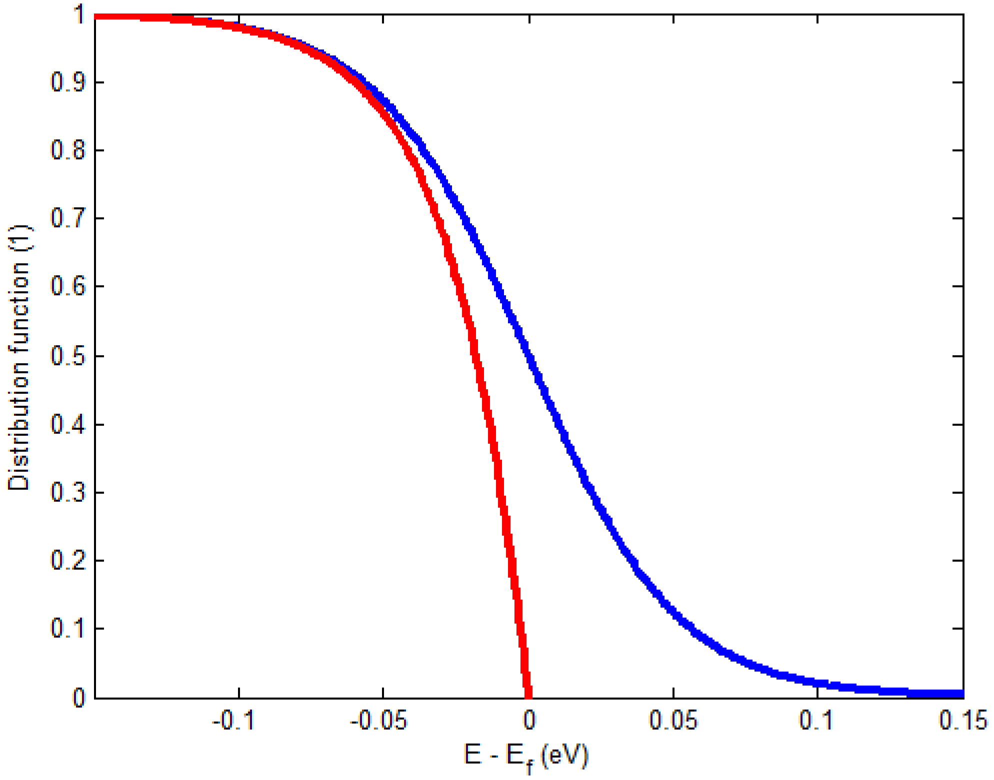


Another Boltzmann limit

- When $E < E_f$,

$$f_D(E) \approx 1 - \exp\left(\frac{E - E_f}{k_B T}\right)$$

Taur, Eq. (2.6)



Carrier concentration (Electron)

- Recall that

Spin and valley degeneracy

$$n = \int_{E_C}^{\infty} N(E) f(E) dE$$

$$N(E) = 2g \frac{4\pi}{h^3} (2m_l m_t^2)^{0.5} (E - E_c)^{0.5}$$

$$f_D(E) = \exp\left(-\frac{E - E_f}{k_B T}\right)$$

– Collecting them all,

$$n = \frac{8\pi g}{h^3} (2m_l m_t^2)^{0.5} \int_{E_C}^{\infty} (E - E_c)^{0.5} \exp\left(-\frac{E - E_f}{k_B T}\right) dE$$

Taur, Eq. (2.8)

Manipulation

- It is found that

$$n = \frac{8\pi g}{h^3}(2m_l m_t^2)^{0.5}\exp\left(-\frac{E_c - E_f}{k_B T}\right) \times \int_{E_c}^{\infty}(E - E_c)^{0.5}\exp\left(-\frac{E - E_c}{k_B T}\right)dE$$

  - Integral can be evaluated as

$$\int_{E_c}^{\infty}(E - E_c)^{0.5}\exp\left(-\frac{E - E_c}{k_B T}\right)dE = (k_B T)^{1.5}\int_{0}^{\infty} z^{0.5}\exp(-z)\,dz = (k_B T)^{1.5}\frac{\sqrt{\pi}}{2}$$

Effective DOS

- Now we know that

$$n = 2g\left(\frac{2\pi k_B T}{h^2}\right)^{1.5}(m_l m_t^2)^{0.5}\exp\left(-\frac{E_c - E_f}{k_B T}\right)$$

  - With the effective DOS,

Dimension?

$$N_c = 2g\left(\frac{2\pi k_B T}{h^2}\right)^{1.5}(m_l m_t^2)^{0.5} \qquad \text{Taur, Eq. (2.10)}$$

  - The electron density can be simply written as

$$n = N_c \exp\left(-\frac{E_c - E_f}{k_B T}\right) \qquad \text{Taur, Eq. (2.9)}$$

  - Following a similar derivation, $p = N_v \exp\left(\frac{E_v - E_f}{k_B T}\right)$ Taur, Eq. (2.11)

Intrinsic carrier concentration

- In this case, $n = p$. Then, what is E_f?

$$N_c \exp\left(-\frac{E_c - E_f}{k_B T}\right) = N_v \exp\left(\frac{E_v - E_f}{k_B T}\right)$$

  - From the above equation,

$$E_f = \frac{E_c + E_v}{2} - \frac{k_B T}{2} \ln \frac{N_c}{N_v}$$

Taur, Eq. (2.12)

  - This energy level is called the intrinsic Fermi level, E_i.
  - In this case,

$$n = p = n_i = \sqrt{N_c N_v} \exp\left(-\frac{E_c - E_v}{k_B T}\right)$$

Using the intrinsic carrier density,

- Carrier densities are expressed as

$$n = n_i \exp\left(-\frac{E_i - E_f}{k_B T}\right)$$ Taur, Eq. (2.14)

$$p = n_i \exp\left(\frac{E_i - E_f}{k_B T}\right)$$ Taur, Eq. (2.15)

  – A useful, general relationship is that the product

$$np = n_i^2$$ Taur, Eq. (2.16)

  in equilibrium is a constant, independent of the Fermi level position.

Thank you!